

Fermi-Dirac Integrals in terms of Zeta Functions

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Abstract

This paper shows the Fermi-Dirac Integrals $F_{\frac{1}{2}}(\eta)$ and $F_{\frac{3}{2}}(\eta)$ expressed in terms of Riemann and Hurwitz Zeta functions. This is done by defining an auxiliary function that permits rewrite the Fermi-Dirac integral in terms of simpler and known integrals resulting in the Zeta functions mentioned. The approach used here evades the use of iterative methods for the integrals and presents a clever procedure for around $\eta \leq 5$, complementing Sommerfeld lemma, one that can be generalized for any integer k in $F_{\frac{k}{2}}(\eta)$ in the refereed interval.

1 Introduction.

The motivation of this paper is to find expressions in order to calculate The Fermi-Dirac integrals specifically for $\eta \leq 5$, values that so far had been calculated using iterative methods as the trapezoidal method, [5]. This integrals appears in partial degenerate stars, [2], thermal conductions by electrons [4], and condensed matter physics. The Fermi-Dirac integral $F_{\frac{k}{2}}(\eta)$ is defined by

$$F_{\frac{k}{2}}(\eta) = \int_0^\infty \frac{\xi^{\frac{k}{2}}}{1 + e^{\xi - \eta}} d\xi \quad (1)$$

Where $\eta = \frac{\mu}{k_B T}$, k_B is the Boltzmann constant and μ the chemical potential.

In this paper we focus on the Fermi-Dirac integral $F_{\frac{1}{2}}(\eta)$, and the procedure and result can be extended to the $F_{\frac{3}{2}}(\eta)$ and generalized for any integer k in equation (1). This procedure involves an auxiliary function that relates $F_{\frac{1}{2}}(\eta)$ with $F_{\frac{1}{2}}(0)$, and based on their (graphical) relation will permit to write the auxiliary function in simple terms and make the integral $F_{\frac{1}{2}}(\eta)$ easier to calculate obtaining Riemann and Hurwitz Zeta functions. That is, with almost no need for iterative methods.

2 Fermi-Dirac $F_{\frac{1}{2}}(\eta)$ and the auxiliary function

As we mentioned, we work on the Fermi-Dirac integral $F_{\frac{1}{2}}(\eta)$, defined by

$$F_{\frac{1}{2}}(\eta) = \int_0^\infty \frac{\xi^{\frac{1}{2}}}{1 + e^{\xi-\eta}} d\xi \quad (2)$$

Actually, we focus on the term defined here by $f_{\frac{1}{2}}(\xi, \eta)$:

$$f_{\frac{1}{2}}(\xi, \eta) = \frac{\xi^{\frac{1}{2}}}{1 + e^{\xi-\eta}} \quad (3)$$

and define the function $f_{\frac{1}{2}}(\xi)$:

$$f_{\frac{1}{2}}(\xi) = \frac{\xi^{\frac{1}{2}}}{1 + e^\xi} \quad (4)$$

We define a function, denoted as $f(\xi, \eta)$, that is the ratio of both functions:

$$f(\xi, \eta) = \frac{f_{\frac{1}{2}}(\eta)}{f_{\frac{1}{2}}(0)} = \frac{1 + e^\xi}{1 + e^{\xi-\eta}} \quad (5)$$

this function, graphically, behaves as $a - be^{-c\xi}$ for $\eta \leq 5$. That is, we assume that we can model and define the function $f(\xi, \eta)$ as:

$$f(\xi, \eta) = a - be^{-c\xi} \quad (6)$$

where a, b, and c are constants. The a and b can be found considering some aspects of equation (5):

$$f(0, \eta) = \frac{2}{1 + e^{-\eta}}$$

and

$$\lim_{x \rightarrow \infty} f(0, \eta) = e^\eta$$

this implies that $a = e^\eta$ and $b = \frac{e^\eta - 1}{e^{-\eta} + 1}$. This means that

$$f(\xi, \eta) = e^\eta - \frac{e^\eta - 1}{e^{-\eta} + 1} e^{-c\xi} \quad (7)$$

This leaves the issue of finding c . We take the following approach, perhaps the only one in this procedure that needs iterative methods: we find the maximum of $f_{\frac{1}{2}}(\xi, \eta)$, equation (3). That is, after the algebra, we must solve for ξ in:

$$e^\eta + e^\xi(1 - 2\xi) = 0 \quad (8)$$

and call this value ξ_m , that depends on η . Using equations (5) and (7), and substituting ξ_m , we can solve for c :

$$c = -\frac{1}{\xi_m} \ln \left[\frac{(e^{-\eta} + 1) \left(e^\eta - \frac{1+e^{\xi_m}}{1+e^{\xi_m-\eta}} \right)}{e^\eta - 1} \right] \quad (9)$$

It can be shown that calculating the two maximums, of equation (3) and $f(\xi, \eta) * f_{\frac{1}{2}}(\xi)$ will lead basically to the same result. Having found the constants in equation (6), we can write equation (2) as follows:

$$\begin{aligned} \int_0^\infty \frac{\xi^{\frac{1}{2}}}{1+e^\xi} d\xi &= \int_0^\infty \left(e^\eta - \frac{e^\eta - 1}{e^{-\eta} + 1} e^{-c\xi} \right) \frac{\xi^{\frac{1}{2}}}{1+e^\xi} d\xi \\ &= e^\eta \int_0^\infty \frac{\xi^{\frac{1}{2}}}{1+e^\xi} d\xi - \frac{e^\eta - 1}{e^{-\eta} + 1} \int_0^\infty \frac{e^{-c\xi} \xi^{\frac{1}{2}}}{1+e^\xi} d\xi \end{aligned}$$

where the first integral in the equality we know from Arfken,[1], can be written as:

$$\int_0^\infty \frac{\xi^{\frac{1}{2}}}{1+e^\xi} d\xi = \Gamma\left(\frac{3}{2}\right) \left(1 - 2^{-\frac{1}{2}}\right) \zeta\left(1 + \frac{1}{2}\right)$$

where $\zeta(p)$ is the well known Riemann Zeta function. For the second integral, after expanding some terms:

$$\begin{aligned} \int_0^\infty \frac{e^{-c\xi} \xi^{\frac{1}{2}}}{1+e^\xi} d\xi &= \Gamma\left(\frac{3}{2}\right) \sum_{n=0}^\infty \frac{(-1)^n}{(c+1+n)^{1+\frac{1}{2}}} \\ &= \Gamma\left(\frac{3}{2}\right) \left[2^{-\frac{1}{2}} \zeta\left(1 + \frac{1}{2}, \frac{c+1}{2}\right) - \zeta\left(1 + \frac{1}{2}, c+1\right) \right] \end{aligned}$$

In the last equality we recognize $\zeta(p, q)$ as the Hurwitz Zeta function, where we used the identity as appears in Williams & Nan-yue, [6]. With these results, we can finally write $F_{\frac{1}{2}}(\eta)$ as:

$$F_{\frac{1}{2}}(\eta) = \Gamma\left(\frac{3}{2}\right) \left[e^\eta \left(1 - 2^{-\frac{1}{2}}\right) \zeta\left(1 + \frac{1}{2}\right) - \frac{e^\eta - 1}{e^{-\eta} + 1} \left[2^{-\frac{1}{2}} \zeta\left(1 + \frac{1}{2}, \frac{c+1}{2}\right) - \zeta\left(1 + \frac{1}{2}, c+1\right) \right] \right] \quad (10)$$

3 Some results

Using equation (10), we elaborate in Table 1, for some η , a comparison with values taken from [2], which were based on McDougall & Stoner, *Phil. Trans. Roy. Soc.*, **237**:67(1938), including some values for positive $\eta < 1$, used in electron conduction opacity, [4], showing how reliable and potentially applicable this method is.

Table 1: $F_{\frac{1}{2}}(\eta)$ values comparison

η	$F_{\frac{1}{2}}$ eq. (10)	$F_{\frac{1}{2}}$ Clayton	error (%)
-4	0.0161393	0.0161277	0.0715548
-3	0.0434453	0.0433664	0.181969
-2	0.11506	0.114588	0.411671
-1	0.292405	0.290501	0.655385
0	0.678094	0.678094	6.95512E-11
.1	0.732034	.733403	0.18664
.5	0.977945	.990209	1.23858
1	1.35129	1.39638	3.22903
2	2.30003	2.50246	8.08906
3	3.58315	3.97699	9.90297
4	5.5495	5.77073	3.83358
5	8.99919	7.83798	14.8152

4 Observations

For $\eta = 1$, the approach here presented is an improvement for the Trapezoidal scheme, [5], where their method gives an 6.4% error. The model according to equation (6) is reliable for $\eta \leq 5$, specially with negative η . Yet, as the ratio of the functions in equation (5) shows a higher inflexion point, for $\eta > 5$, the model needs an improvement. The reason for the limitation around this value appears when analyzing the equation (10), where a simple examination shows a dependency of order e^η , as it happens in Sommerfeld lemma.

5 Conclusion

The equation (10) gives an expression for calculating the Fermi-Dirac integrals $F_{\frac{1}{2}}(\eta)$ in terms of the Riemann and Hurwitz Zeta functions. Using the same procedure we find expressions for $F_{\frac{3}{2}}(\eta)$ and $F_{\frac{k}{2}}(\eta)$, for general integer k , valid for $\eta \leq 5$. This approach complements that of Sommerfeld lemma, giving a nearly complete expression for Fermi-Dirac integrals.

$$F_{\frac{3}{2}}(\eta) = \Gamma\left(\frac{5}{2}\right) \left[e^{\eta} \left(1 - 2^{-\frac{3}{2}}\right) \zeta\left(1 + \frac{3}{2}\right) - \frac{e^{\eta} - 1}{e^{-\eta} + 1} \left[2^{-\frac{3}{2}} \zeta\left(1 + \frac{3}{2}, \frac{c+1}{2}\right) - \zeta\left(1 + \frac{3}{2}, c+1\right) \right] \right] \quad (11)$$

and for general k:

$$F_{\frac{k}{2}}(\eta) = \Gamma\left(1 + \frac{k}{2}\right) \left[e^{\eta} \left(1 - 2^{-\frac{k}{2}}\right) \zeta\left(1 + \frac{k}{2}\right) - \frac{e^{\eta} - 1}{e^{-\eta} + 1} \left[2^{-\frac{k}{2}} \zeta\left(1 + \frac{k}{2}, \frac{c+1}{2}\right) - \zeta\left(1 + \frac{k}{2}, c+1\right) \right] \right] \quad (12)$$

with the remark that ξ_m , equation (8), in order to find c (notice that c and $f(\xi, \eta)$ are k-independent), must be generalized too:

$$ke^{\eta} + e^{\xi}(k - 2\xi) = 0 \quad (13)$$

References

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